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**X_x-X_{xy} crossover in a two-dimensional electron gas in AlAs**

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Received 16 June 1995; accepted for publication 2 August 1995

**Abstract**

We have performed magnetoresistance measurements up to 20 T on high-mobility two-dimensional electron gases in single AlAs quantum wells with well widths ranging from 40 to 80 Å. We observe a sharp transition from a two-fold valley degenerate X_{xy} occupied state in a 60 Å well to a non-degenerate X_x occupied state in a 40 Å well. These two states are distinguished by their different effective masses, which have been determined using the temperature dependence of the Shubnikov-de Haas effect. Using self-consistent calculations, we can explain this transition in relative occupation assuming an X-splitting energy of 24 meV. Furthermore, for the X_x electrons, the effect of the large ratio of spin to Landau splitting is shown by the occurrence of strong magnetoresistance minima at filling factors 2, 6 and 10 in the Hall effect.

**Keywords:** Aluminum arsenide; Effective masses; Electrical transport measurements; Gallium arsenide; Hall effect; Quantum wells; Superlattices

1. Introduction

Although AlAs is commonly used in superlattices (SL) and as a barrier material in heterostructures, its electrical parameters are only infrequently studied. This is mainly due to the fact that AlAs is an indirect semiconductor, having the X minimum as the lowest conduction-band minimum, and confining these X electrons to a 2DEG is difficult. The equi-energy surfaces at this X minimum are strongly non-isotropic in k space and are described by different longitudinal and transverse effective masses m_l and m_t. The minimum has a three-fold degeneracy, denoted by X_x, X_y, and X_z. In a two-dimensional system the X_x and X_y valleys remain degenerate, denoted by X_{xy}, whereas the degeneracy with the X_z minimum is lifted.

The band-structure parameters of AlAs become apparent in short-period type II GaAs_a/AlAs_m SLs. In optically detected magnetic resonance measurements it is found that in these SLs, the lowest X state changes from X_{xy} character to X_x character if the AlAs thickness becomes smaller than 55 Å [1]. Cyclotron resonance measurements and recent Shubnikov–de Haas measurements [2–4] revealed the density of states (DOS) effective masses of these states, m_{xy} = \sqrt{(m_l m_t)} = 0.5–0.6m_0 and m_x = m_t = 0.3m_0. Apparently, for wide wells, the energy position of the X_{xy} and X_x states is reversed with respect to what is expected from the binding masses m_l and m_t (≈ 1.0m_0). It is commonly
accepted that this level reversal is caused by the small but finite strain in the AlAs layer induced by the lattice mismatch between GaAs and AlAs \[5\]. The strain-induced energy splitting ranges from 19 to 23 meV \[1,6\].

Up to now the DOS effective masses of the X minimum have only been determined in low-mobility quasi-two-dimensional electron gases (2DEG) in multiple quantum well (QW) structures, where the barrier material itself is indirect (e.g. Al\(_x\)Ga\(_{1-x}\)As with \(x>0.37\)) \[4,7\]. The disadvantage of a multiple QW system is the unknown number of active wells and the non-uniformity of the 2DEG. The use of AlGaAs as a barrier material, makes comparison with optical measurements on the GaAs/AlAs SLs more difficult. Lay \[8\] used a single AlAs/AlGaAs QW, but determined only the cyclotron mass of the X\(_\gamma\) state and its two-fold degeneracy.

In this paper we present a different structure, in which we overcome the aforementioned problems. We have designed a single AlAs QW embedded between five periods of a 22 \AA\/11 \AA\ GaAs/AlAs SL. Two buffer layers of Al\(_{0.37}\)Ga\(_{0.63}\)As (0.1 \(\mu\)m) terminate the SLs. The structure is capped by a thick GaAs (0.5 \(\mu\)m) layer to provide the acceptor background charges to accommodate the surface-band bending, and to make the structure symmetrical. The X-band structure is sketched in Fig. 1. The thickness of the GaAs and AlAs layers in the SL is chosen such that the bound \(\Gamma\) and X states are much higher in energy (~100 meV) than the bottom of the AlAs well. Free carriers are provided by \(\delta\)-doping one of the GaAs layers in the SL on each side of the well. By doping the GaAs we avoid trapping of electrons by the DX centre. Due to the band bending, the Fermi level in the SL is lifted with respect to the centre of the AlAs well and may therefore reach the \(\Gamma\) and X levels in the SL if the total doping density is too high, or if the distance from the \(\delta\)-layer to the well is too large. By fine-tuning the design of our structures we were able to obtain a 2DEG with a single occupied sub-band populated up to \(1.5 \times 10^{12} \text{ cm}^{-2}\).

2. Experimental

Using MBE, we have grown structures at 600\(^\text{o}\)C with well widths of 40, 60 and 80 \(\AA\), and a total Si doping concentration of \(2 \times 10^{12} \text{ cm}^{-2}\). The growth temperature was deliberately lower than the optimum growth temperature of a GaAs/AlAs SL in order to suppress diffusion of Si. Electrical measurements were performed on Hall-bar etched samples with Sn diffused contacts. The characterisation data is given in Table 1. The 40 \(\AA\) well with an X\(_\gamma\)-like 2DEG has the highest mobility reported so far, and demonstrates the high quality of our samples.

Magnetoresistance measurements up to 20 T were performed, and effective masses were determined from the temperature dependence of the SdH oscillations \[9\]. By pumping a \(^4\)He bath cryostat, the temperature was varied between 4.2 K and 1.5 K. Additional temperature reduction to 0.5 K could be obtained in a \(^3\)He cryostat. The relative amplitude variation of an SdH maximum (minimum) has been measured with respect to a line tangential to the adjacent SdH minima (maxima). This method eliminates the effect of background in the magnetoresistance. Effective masses were determined in this way for magnetic fields up to ~6 T. Beyond this magnetic field, the oscillation amplitudes become too large and the
spin- and valley-splitting cannot be neglected. This results in absurd values for the effective mass. The DOS effective masses and their degeneracy have been determined for all well thicknesses and are presented in Table 1.

### Table 1
Sample parameters for our single AlAs QW structures. Sample S80 was grown with the δ-layer in either the (a) second or (b) third GaAs layer of the SL

<table>
<thead>
<tr>
<th>Sample</th>
<th>AlAs well width (Å)</th>
<th>Distance from δ-layer to centre well (Å)</th>
<th>$n_{\text{Fermi}}$ ($10^{12}$ cm$^{-2}$)</th>
<th>$n_{\text{eff}}$ ($10^{12}$ cm$^{-2}$)</th>
<th>$\mu_{\text{Hall}}$ (cm$^2$/V·s)</th>
<th>DOS effective mass ($m_0$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S40</td>
<td>40</td>
<td>65</td>
<td>1.26</td>
<td>1.19</td>
<td>3700</td>
<td>0.27 ± 0.03</td>
</tr>
<tr>
<td>S60</td>
<td>60</td>
<td>75</td>
<td>1.25</td>
<td>0.63</td>
<td>4100</td>
<td>0.64 ± 0.03</td>
</tr>
<tr>
<td>S80$^a$</td>
<td>80</td>
<td>85</td>
<td>0.91</td>
<td>0.52</td>
<td>1700</td>
<td>0.48 ± 0.02</td>
</tr>
<tr>
<td>S80$^b$</td>
<td>80</td>
<td>120</td>
<td>1.06</td>
<td>0.54</td>
<td>7100</td>
<td>0.63 ± 0.02</td>
</tr>
</tbody>
</table>

3. Results and discussion

The striking difference between samples S40 and S80$^b$ is shown in Fig. 2. In both wells only one subband is occupied, which simplifies the interpretation of the measurements. The effective mass measurements indicate that S40 is occupied by $X_z$ electrons and S80 by $X_{xy}$ electrons. Sample S60 shows a similar behaviour to sample S80$^b$. The degeneracy follows from the ratio of the density obtained from the SdH periods at low magnetic fields and the density obtained from the Hall resistance. The degeneracy, excluding spin degeneracy, is 1 for the $X_z$ and 2 for the $X_{xy}$ electrons. The two-fold degeneracy of the $X_{xy}$ state is supported by the successive strong magnetoresistance minima at filling factors $v=2,6$ and 10. This sequence is explained by a large ratio of the spin to Landau splitting,

$$\alpha = g^* \mu _{\text{B}} / \hbar \omega _0 = \frac{1}{2} g^* m^*/m_0,$$

where $g^*$ is the effective $g$ factor (≈ 3 in this system [7]). Thus for this type of electrons, the spin- and Landau-splitting are of comparable size ($\alpha \approx 0.9$). This causes the valley degenerate spin-states of two adjacent Landau levels to join each other, resulting in an effective four-fold degeneracy. At high magnetic fields the degeneracy of such a set of levels is lifted, and magnetoresistance minima at filling factors $v=3, 4$, and 5 are resolved.

Samples S60 and S80$^b$, with the δ-layer in the

Fig. 2. Magnetoresistance and Hall resistance of samples (a) S40 and (b) S80$^b$ at 0.7 K. The filling factors at the magnetoresistance minima are indicated.
second and third GaAs layers of the SL, respectively, have a comparable effective mass of \( \sim 0.63m_0 \). Sample S80\(^a\), however, gives a much lower value of 0.48\(m_0\). These values cover the range of values determined by temperature-dependent SdH measurements in the literature [4,7]. Note that we have indications that the sample quality of S80\(^a\) is much poorer than S80\(^b\). The effective mass measured for the \( X \) electrons (0.27\(m_0\)) is identical to that found by Yamada et al. [4].

Our measurements indicate that the transition region of crossover from an \( X_z \) state to an \( X_{xy} \) populated state is very sharp and occurs between 40 and 60 Å. We have modelled our structures by solving the Schrödinger and Poisson equations in a self-consistent way. The model incorporates the conservation of probability flux at the GaAs/AlAs interfaces (e.g. \( 1/m^*_GaAs \partial \varphi_{GaAs}/\partial z = 1/m^*_AlAs \partial \varphi_{AlAs}/\partial z \)).

Commonly accepted material parameters have been used for GaAs and AlAs. The transition region of the relative occupation change from \( X_z \) to \( X_{xy} \) can best be described by taking an \( X \) splitting energy of 24 ± 2 meV, which is comparable to the value of van Kesteren et al. [1] (Fig. 3a). The crossover in relative occupation of the \( X_z \) and \( X_{xy} \) states occurs at \( \sim 48 \) Å and does not coincide with the crossover of the confinement energies in the well (\( E_x, E_y \)) as shown in Fig. 3b. If we compare this crossover of \( E_x \) and \( E_y \) for doped and undoped wells, we have to conclude that the shift towards lower well-widths of the crossover in relative occupation depends largely upon the different DOS in the \( X_z \) and \( X_{xy} \) levels.

![Image](image_url)

**Fig. 3.** (a) The relative occupation of the \( X_{xy} \) electrons as a function of well width for various strain-induced energy splittings of the \( X_z \) and \( X_{xy} \) levels at a doping concentration of \( 1.25 \times 10^{12} \) cm\(^{-2}\). Our measurements are indicated by dots. (b) The crossover in energy position for (○) undoped and (□) doped structures, and (▽) the relative occupation as a function of the strain-induced energy splitting.

masses of different samples with the same well width, which is not yet understood.

### 4. Summary

We have demonstrated the \( X_z-X_{xy} \) crossover in a high-quality 2DEG in a single AlAs QW and determined the effective masses and their degeneracy. A longitudinal effective mass of 1.5\(m_0\) and a transverse effective mass of 0.3\(m_0\) have been found, which are comparable to the values found in the literature. In addition, the effect of a large ratio of spin- to Landau-splitting has been shown. There is, however, a discrepancy between the effective

### References